PUBCHEM_54609806

3698-87-1 | DTXSID60715027

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: -11.1 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 2.71e-01

Confidence level: 8.38e-01

Nearest Neighbors from the Training Set

Image not found
Bornyl acetate
Measured: -10.9
Predicted: -10.9

Image not found
Ethyl lactate
Measured: -11.4
Predicted: -11.3

Image not found
2-Ethoxyethyl isobutyrate
Measured: -10.9
Predicted: -10.9

Image not found
Ethyl 3-ethoxypropionate
Measured: -10.6
Predicted: -10.8

Image not found
Methyl 2-hydroxypropanoate
Measured: -11.6
Predicted: -11.5